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THE UNITED STATES PATENT AND TRADEMARK OFFICE

GROUP ART UNIT 1744

Examiner: F. Varcoe, Jr.

February __, 2001



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I am an employee of Shell International Exploration and Production, Inc., an affiliate of Shell Oil Company, a corporation organized and existing under the laws of the state of Delaware, having a place of business at One Shell Plaza, 910 Louisiana, Houston, TX 77252.

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search
or

I began working for Shell Development Company in 1991 as an Associate Research Engineer in the area of reaction engineering, with experience in reaction kinetics, reactor modeling and optimization, process development, design and scale-up, and reactive hazards assessment. I officially joined Shell International Exploration and Production, Inc. the beginning of this year.

I have worked with the inventors of the process described in above-identified U. S. Patent Application Ser. No. 09/168,770 and am very familiar with that process and its applications.

I modified a rigorous reactor model written in FORTRAN with thousands of lines of code to predict how intermediate reheat with Flameless Distributed Combustion (Hereafter referred to as FDC) tubes inside a reactor would affect the first reactor stage conversion and capacity. This model, named STYRENE, accounts for homogeneous and heterogeneous kinetics, diffusional limitations, catalyst deactivation, and pressure drop. The model performs heat and mass balances in each reactor stage and the preheat zones. The model can also regress pilot or plant

data to determine best kinetic parameters. R. Hawthorn developed the model 20 years ago at Shell's Westhollow Technology Center and it has been improved by L. A. Clomburg and myself. This is an established model used, for example, by Criterion Catalyst Company to make plant performance predictions.

I used the model to predict how intermediate reheat with FDC tubes inside the reactor, as described in Claim 1 of Ser. No. 09/168,770, as applied to the manufacture of styrene, as described beginning at page 12, last two lines of the application, would affect first stage conversion and capacity.

I found that the increase of the conversion was from 40.1% to 58.5%, leading to ca. 46% higher first stage capacity, and only 12% less than the two-stage conventional train. This result indicates that the second reactor which ordinarily achieves a cumulative conversion of 66.5% would not be necessary, since the capacity of the first stage with FDC tubes would approach the total capacity of the conventional reactors.

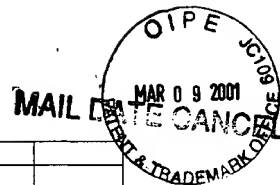
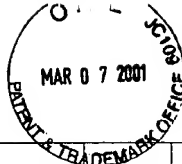
A copy of the input file for the reactor model is attached as Exhibit A. (Input file for styrene FORTRAN model). Exhibit B is data for the profile of the reactors.

Model results for an isothermal reactor are attached as Exhibit C and model results for a non-isothermal reactor are attached as Exhibit D. Exhibit E describes input on membrane design, mass and heat balances, however in the STYRENE model no hydrogen was actually removed from the process side of the modeling; therefore, the elements present were representative of the use of the process of Ser. No. 09/168,770 as an oxidation reaction chamber in the production of styrene.

I modeled two adiabatic radial flow reactors (notional segments) with the same length of 11.57m and the ID and OD's of (1.6, 2.5) m and (2.5, 3.14) m respectively, with reheat to the same inlet temperature of 608°C.

Geometry data for the modeled reactor is as follows: Table 1
Number reactor stages = 2
Unit = LG Chemical Korea
Reactor types:
1= Isothermal, axial 2= adiabatic, axial 3= adiabatic, radial

Press
description



Reactor Number	Reactor type	Catalyst number	Catalyst activity	Bed void fraction	bed dimensions, cm			bed inlet vol, m ³	
					Bed length, cm	bed inner radius, cm	bed outer radius, cm		
1	3	6	1.000	.370	1157.	80.	125.	9.49	
2	3	6	1.000	.370	1157.	125.	157.	0.00	

I summarized the key data in the following table:

Exhibit B: Table 2

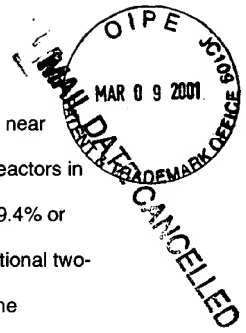
Radial Reactor Case	1 st stage conversion and STY selectivity	2 nd stage conversion and STY selectivity	Number of 1 inch tubes needed	Percent of equilibrium constant (1 st , 2 nd)
1. Adiabatic (no H ₂ removal)	40.14% w/ 97.39%	66.46% w/96.71%	NA	24.1%, 18.9% (no equil. limit)
2. Adiabatic with mid-volume reheat (no H ₂ removal)	58.49% w/ 97.22% (35.3% in the first half of the volume)	Not done	33-214 (optimistic vs. current)	41.7%, NA
3. Adiabatic with mid-volume reheat (with H ₂ removal)	Model does not allow, but greater than #2	Not done	>33-214	30.1%, NA
4. Isothermal (no H ₂ removal)	79.42% w/ 95.24%	87.67% w/93.56%	57-370 (optimistic vs. current)	61.6%, 53.1% (closer to equil. limit; max =100%)
5. Isothermal (with H ₂ removal)	Model does not allow, but greater than #4	Model does not allow, but greater than #2	>57-370	32.7%, 50.4% (further from limit)

The process of Ser. No. 09/168,770 used in the production of styrene provides surprising results and overwhelming advantages which would not have been apparent to one skilled in the art by observing Minet et al. in view of Mikus.

The reaction model shows that when the FDC of Ser. No. 09/168,770 is employed in an endothermic reaction the following surprising results are observed:

- 1) Improved selectivities and/or yields;
- 2) Reduced byproducts due to uniform heat input;
- 3) Reduced hot spots due to the use of FDC;
- 4) Elimination of interstage reheats, thus enabling operation at optimum temperature;
- 5) Even temperature profiles with respect to materials of construction;
- 6) Permits the reactor to function essentially isothermally;
- 7) Permits a considerably higher average temperature because reactor tubes are of uniform temperature.

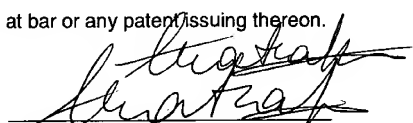
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I was also able to calculate that the modeled reactor can potentially run near isothermally and achieve at least twice or greater the capacity of conventional styrene reactors in one pass. This is demonstrated in Table 2 in which the conversion of the first stage is 79.4% or 98% higher capacity than the conventional one-stage. When compared with the conventional two-stage train, the capacity is still 20% higher, with some small reduction of 2.17% in styrene selectivity. This result again confirms that the second reactor, which ordinarily achieves a cumulative conversion of 66.5%, would not be necessary, since the capacity of the first stage, with the FDC tubes securing isothermal operation, would exceed by 20% the total capacity of the two conventional reactors.

I am also closely involved with the business aspects of this technology and would respectfully assert that further evidence that Ser. No. 09/168,770 would not have been obvious to one skilled in the art observing Minet et al. in view of Mikus is that the Washington Group, formerly Raytheon found that the technology was improved over any similar technology available in the art and filled a distinct need in the art; and, the Washington Group has entered into an exclusive license with Shell to use said technology.

This Affidavit is made with the knowledge that the United States Patent Office will rely on information contained therein, and that willful false statements are punishable by fine or imprisonment or both, under §101 of Title 18 of the United States Code, and that such willful false statements may jeopardize the validity of the application at bar or any patent issuing thereon.


ANDREAS N. MATZAKOS

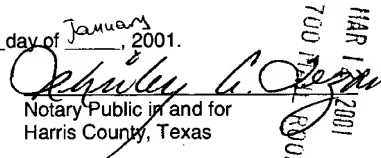
STATE OF TEXAS

§
§
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COUNTY OF HARRIS

Sworn to and subscribed before me this 29 day of January, 2001.




Notary Public in and for
Harris County, Texas

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Exhibit A

Styrene Catalyst Input File
Cataly035 LGC Plant Data
16

Laboratory data table

Rxr-Volu

Oil dens

Inlet %w composition

gas added, Rxr Performance

Weight Factor Matrix

Days oReactorPressureInlet teWater adOil flow EB Styrene Tol

Ben inert CO H2Rrx lenEB ConvS(styreneS(tolueS(benzeTgut, CEB

ConS(tolueS(benzeTgut, Sum (se

00	1		10.10	608.0	1.70	42200.0	98.97	0.40	
0.02	0.0	0.0	0.0	0.00	0.0	0.0	0.0	0.0	628.3
0	0	1	0.0						
00	1		10.10	608.0	1.70	42200.0	98.97	0.40	
0.02	0.0	0.0	0.0	455.50	37.2	98.3	1.2	0.5	559.4
1	1	1	100.0						
00	2		7.30	608.0	0.00	0.0	0.00	0.00	
0.00	0.0	0.0	0.0	0.00	37.2	0.0	0.0	0.0	631.7
0	0	1	0.0						
00	2		7.30	608.0	0.00	0.0	0.00	0.00	
0.00	0.0	0.0	0.0	375.20	63.7	97.5	1.9	0.6	581.7
1	1	1	100.0						
10	1		10.10	608.0	1.70	42200.0	98.97	0.40	0.41
0.02	0.0	0.0	0.0	0.00	0.0	0.0	0.0	0.0	628.3
0	0	1	0.0						
10	1		10.10	608.0	1.70	42200.0	98.97	0.40	0.41
0.02	0.0	0.0	0.0	455.50	36.9	98.2	1.2	0.6	559.4
1	1	1	100.0						
10	2		7.30	608.0	0.00	0.0	0.00	0.00	
0.00	0.0	0.0	0.0	0.00	36.9	0.0	0.0	0.0	631.7
0	0	1	0.0						
10	2		7.30	608.0	0.00	0.0	0.00	0.00	
0.00	0.0	0.0	0.0	375.20	63.0	97.8	1.8	0.4	581.1
1	1	1	100.0						
20	1		10.10	608.0	1.70	42200.0	98.97	0.40	0.41
0.02	0.0	0.0	0.0	0.00	0.0	0.0	0.0	0.0	628.3
0	0	1	0.0						
20	1		10.10	608.0	1.70	42200.0	98.97	0.40	0.41
0.02	0.0	0.0	0.0	455.50	35.7	98.2	1.3	0.6	559.8
1	1	1	100.0						
20	2		7.30	608.0	0.00	0.0	0.00	0.00	
0.00	0.0	0.0	0.0	0.00	35.7	0.0	0.0	0.0	632.8
0	0	1	0.0						
20	2		7.30	608.0	0.00	0.0	0.00	0.00	
0.00	0.0	0.0	0.0	375.20	61.9	97.7	1.7	0.6	581.3
1	1	1	100.0						
105	1		10.10	608.0	1.70	42200.0	98.97	0.40	0.41
0.02	0.0	0.0	0.0	0.00	0.0	0.0	0.0	0.0	628.3
0	0	1	0.0						
105	1		10.10	608.0	1.70	42200.0	98.97	0.40	0.41
0.02	0.0	0.0	0.0	455.50	35.9	97.9	1.4	0.7	561.7
1	1	1	100.0						
105	2		7.30	608.0	0.00	0.0	0.00	0.00	
0.00	0.0	0.0	0.0	0.00	35.9	0.0	0.0	0.0	633.3
0	0	1	0.0						
105	2		7.30	608.0	0.00	0.0	0.00	0.00	
0.00	0.0	0.0	0.0	375.20	62.0	97.5	1.8	0.6	581.9
1	1	1	100.0						
123	1		11.17	628.3	1.40	42200.0	96.23	1.25	0.45
0.32	0.0	0.0	0.0	0.00	0.0	0.0	0.0	0.0	628.3
0	0	1	0.0						
123	1		10.68	628.3	1.40	42200.0	96.23	1.25	0.45
0.32	0.0	0.0	0.0	30.00	35.7	98.1	1.2	0.7	560.7



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1	1	1	100.0							
123	2		7.09	633.9	0.00	0.0	0.00	0.00	0.00	0.00
0.00	0.0	0.0	0.0	0.00	35.7	0.0	0.0	0.0	633.9	1
0	0	1	0.0							
123	2		6.15	633.9	0.00	0.0	0.00	0.00	0.00	0.00
0.00	0.0	0.0	0.0	30.00	61.6	97.7	1.7	0.6	581.8	1
1	1	1	100.0							
154	1		11.21	628.9	1.411271	120.0	96.15	1.22		0.45
0.29	0.0	0.0	0.0	0.00	0.0	0.0	0.0	0.0	628.9	1
0	0	1	0.0							
154	1		11.21	628.9	1.411271	120.0	96.15	1.22		0.45
0.29	0.0	0.0	0.0	30.00	35.6	97.9	1.3	0.8	562.1	1
1	1	1	100.0							
154	2		7.15	634.4	0.00	0.0	0.00	0.00	0.00	0.00
0.00	0.0	0.0	0.0	0.00	35.6	0.0	0.0	0.0	634.4	1
0	0	1	0.0							
154	2		7.15	634.4	0.00	0.0	0.00	0.00	0.00	0.00
0.00	0.0	0.0	0.0	30.00	61.5	97.6	1.7	0.7	582.3	1
1	1	1	100.0							
169	1		11.46	629.4	1.481257	58.0	96.90	1.04		0.35
0.30	0.0	0.0	0.0	0.00	0.0	0.0	0.0	0.0	629.4	1
0	0	1	0.0							
169	1		11.46	629.4	1.481257	58.0	96.90	1.04		0.35
0.30	0.0	0.0	0.0	30.00	37.5	97.7	1.4	0.9	558.4	1
1	1	1	100.0							
169	2		7.40	635.1	0.00	0.0	0.00	0.00	0.00	0.00
0.00	0.0	0.0	0.0	0.00	37.5	0.0	0.0	0.0	635.1	1
0	0	1	0.0							
169	2		7.40	635.1	0.00	0.0	0.00	0.00	0.00	0.00
0.00	0.0	0.0	0.0	30.00	66.0	96.8	2.2	1.0	580.6	1
1	1	1	100.0							
193	1		11.37	629.4	1.411262	10.0	95.92	1.40		0.46
0.34	0.0	0.0	0.0	0.00	0.0	0.0	0.0	0.0	629.4	1
0	0	1	0.0							
193	1		11.37	629.4	1.411262	10.0	95.92	1.40		0.46
0.34	0.0	0.0	0.0	30.00	34.9	98.1	0.8	1.1	563.6	1
1	1	1	100.0							
193	2		7.32	635.0	0.00	0.0	0.00	0.00	0.00	0.00
0.00	0.0	0.0	0.0	0.00	34.9	0.0	0.0	0.0	635.0	1
0	0	1	0.0							
193	2		7.32	635.0	0.00	0.0	0.00	0.00	0.00	0.00
0.00	0.0	0.0	0.0	30.00	61.3	97.2	1.8	0.9	583.6	1
1	1	1	100.0							
216	1		11.34	630.0	1.401262	10.0	96.63	1.30		0.45
0.29	0.0	0.0	0.0	0.00	0.0	0.0	0.0	0.0	630.0	1
0	0	1	0.0							
216	1		10.78	564.3	1.401262	10.0	96.63	1.30		0.45
0.29	0.0	0.0	0.0	30.00	35.3	97.8	1.3	0.9	564.3	1
1	1	1	100.0							
216	2		7.22	635.6	0.00	0.0	0.00	0.00	0.00	0.00
0.00	0.0	0.0	0.0	0.00	35.3	0.0	0.0	0.0	635.6	1
0	0	1	0.0							
216	2		6.21	583.4	0.00	0.0	0.00	0.00	0.00	0.00
0.00	0.0	0.0	0.0	30.00	60.3	97.2	1.9	1.0	583.4	1
1	1	1	100.0							

Exhibit B



Profiles for reactor bed number 1

No Temp Press Concentrations, gmole/kg total feed -----

Effectiveness factors -----

step	DC	Psia	EB	Styrene	Toluene	Benzene	EB = Sty	EB =
Ben	Sty = Tol	Sty = CO2						
0	607.6	10.10	3.451E+00	2.079E-02	1.753E-02	2.138E-03		
1	593.8	10.02	3.183E+00	2.833E-01	2.146E-02	3.340E-03	1.782E-01	
1.809E-01	1.306E+00	1.322E+00						
2	583.7	9.95	2.989E+00	4.737E-01	2.385E-02	4.203E-03	3.263E-01	
3.325E-01	1.037E+00	1.047E+00						
3	576.4	9.88	2.850E+00	6.096E-01	2.555E-02	4.819E-03	4.427E-01	
4.518E-01	9.761E-01	9.828E-01						
4	571.1	9.82	2.749E+00	7.097E-01	2.688E-02	5.276E-03	5.288E-01	
5.403E-01	9.585E-01	9.636E-01						
5	567.0	9.76	2.670E+00	7.867E-01	2.798E-02	5.631E-03	5.936E-01	
6.068E-01	9.534E-01	9.575E-01						
6	563.6	9.70	2.607E+00	8.483E-01	2.892E-02	5.917E-03	6.435E-01	
6.579E-01	9.527E-01	9.561E-01						
7	560.9	9.65	2.555E+00	8.991E-01	2.975E-02	6.155E-03	6.830E-01	
6.983E-01	9.536E-01	9.566E-01						
8	558.6	9.60	2.511E+00	9.420E-01	3.050E-02	6.358E-03	7.149E-01	
7.307E-01	9.552E-01	9.577E-01						
9	556.5	9.56	2.473E+00	9.789E-01	3.119E-02	6.534E-03	7.410E-01	
7.573E-01	9.569E-01	9.592E-01						
10	554.8	9.51	2.440E+00	1.011E+00	3.181E-02	6.689E-03	7.629E-01	
7.793E-01	9.587E-01	9.607E-01						
11	553.2	9.47	2.411E+00	1.040E+00	3.240E-02	6.828E-03	7.813E-01	
7.979E-01	9.604E-01	9.622E-01						
12	551.8	9.43	2.384E+00	1.065E+00	3.294E-02	6.953E-03	7.970E-01	
8.137E-01	9.620E-01	9.636E-01						
13	550.5	9.40	2.361E+00	1.088E+00	3.345E-02	7.067E-03	8.107E-01	
8.274E-01	9.634E-01	9.650E-01						
14	549.4	9.36	2.339E+00	1.109E+00	3.394E-02	7.172E-03	8.225E-01	
8.392E-01	9.648E-01	9.662E-01						
15	548.3	9.32	2.319E+00	1.129E+00	3.440E-02	7.268E-03	8.330E-01	
8.496E-01	9.661E-01	9.674E-01						
16	547.4	9.29	2.301E+00	1.146E+00	3.484E-02	7.358E-03	8.422E-01	
8.587E-01	9.673E-01	9.685E-01						
17	546.4	9.26	2.284E+00	1.163E+00	3.526E-02	7.441E-03	8.504E-01	
8.669E-01	9.684E-01	9.695E-01						
18	545.6	9.23	2.268E+00	1.178E+00	3.566E-02	7.519E-03	8.578E-01	
8.741E-01	9.694E-01	9.705E-01						
19	544.8	9.20	2.253E+00	1.192E+00	3.604E-02	7.592E-03	8.644E-01	
8.807E-01	9.703E-01	9.714E-01						
20	544.1	9.17	2.240E+00	1.205E+00	3.642E-02	7.662E-03	8.704E-01	
8.866E-01	9.712E-01	9.722E-01						

Profiles for reactor bed number 2

No Temp Press Concentrations, gmole/kg total feed -----

Effectiveness factors -----

step	DC	Psia	EB	Styrene	Toluene	Benzene	EB = Sty	EB =
Ben	Sty = Tol	Sty = CO2						
0	608.0	7.30	2.240E+00	1.205E+00	3.642E-02	7.662E-03		
1	600.8	7.26	2.102E+00	1.339E+00	3.904E-02	8.278E-03	4.030E-01	
4.269E-01	8.736E-01	8.804E-01						
2	595.4	7.22	1.998E+00	1.440E+00	4.114E-02	8.748E-03	4.736E-01	
5.019E-01	8.895E-01	8.949E-01						
3	591.2	7.19	1.917E+00	1.520E+00	4.291E-02	9.123E-03	5.299E-01	
5.617E-01	9.020E-01	9.064E-01						
4	587.7	7.15	1.851E+00	1.584E+00	4.444E-02	9.431E-03	5.755E-01	
6.100E-01	9.119E-01	9.157E-01						
5	584.8	7.12	1.796E+00	1.637E+00	4.579E-02	9.692E-03	6.130E-01	

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6.496E-01	9.199E-01	9.232E-01						
6 582.4	7.09	1.749E+00	1.682E+00	4.701E-02	9.916E-03	6.443E-01		
6.825E-01	9.265E-01	9.293E-01						
7 580.3	7.06	1.709E+00	1.721E+00	4.812E-02	1.011E-02	6.708E-01		
7.101E-01	9.319E-01	9.344E-01						
8 578.4	7.02	1.673E+00	1.755E+00	4.915E-02	1.029E-02	6.934E-01		
7.336E-01	9.365E-01	9.387E-01						
9 576.8	6.99	1.642E+00	1.785E+00	5.010E-02	1.045E-02	7.129E-01		
7.538E-01	9.404E-01	9.424E-01						
10 575.3	6.97	1.614E+00	1.812E+00	5.099E-02	1.059E-02	7.299E-01		
7.712E-01	9.438E-01	9.456E-01						
11 573.9	6.94	1.589E+00	1.836E+00	5.183E-02	1.072E-02	7.448E-01		
7.865E-01	9.468E-01	9.484E-01						
12 572.7	6.91	1.566E+00	1.858E+00	5.262E-02	1.084E-02	7.580E-01		
8.000E-01	9.494E-01	9.509E-01						
13 571.6	6.88	1.545E+00	1.878E+00	5.338E-02	1.095E-02	7.697E-01		
8.119E-01	9.517E-01	9.531E-01						
14 570.6	6.85	1.526E+00	1.896E+00	5.410E-02	1.105E-02	7.802E-01		
8.225E-01	9.537E-01	9.551E-01						
15 569.6	6.83	1.508E+00	1.913E+00	5.479E-02	1.115E-02	7.897E-01		
8.320E-01	9.556E-01	9.568E-01						
16 568.8	6.80	1.492E+00	1.929E+00	5.545E-02	1.124E-02	7.982E-01		
8.406E-01	9.573E-01	9.584E-01						
17 567.9	6.78	1.476E+00	1.943E+00	5.608E-02	1.133E-02	8.060E-01		
8.483E-01	9.588E-01	9.599E-01						
18 567.2	6.75	1.462E+00	1.957E+00	5.669E-02	1.141E-02	8.131E-01		
8.554E-01	9.602E-01	9.612E-01						
19 566.5	6.73	1.449E+00	1.970E+00	5.729E-02	1.149E-02	8.196E-01		
8.618E-01	9.615E-01	9.625E-01						
20 565.8	6.71	1.436E+00	1.981E+00	5.786E-02	1.156E-02	8.256E-01		
8.677E-01	9.627E-01	9.636E-01						

Profiles for reactor bed number 1

No	Temp	Press	Concentrations,	gmole/kg total feed	-----			
Effectiveness factors	-----							
step	DC	Psia	EB	Styrene	Toluene	Benzene	EB = Sty	EB =
Ben	Sty	= Tol	Sty = CO2					
0	607.6	10.10	3.451E+00	2.079E-02	1.753E-02	2.138E-03		
1	594.0	10.02	3.188E+00	2.783E-01	2.124E-02	3.317E-03	1.843E-01	
1.869E-01	1.326E+00	1.342E+00						
2	584.1	9.95	2.997E+00	4.655E-01	2.352E-02	4.165E-03	3.315E-01	
3.374E-01	1.047E+00	1.057E+00						
3	577.0	9.88	2.861E+00	5.994E-01	2.514E-02	4.772E-03	4.465E-01	
4.553E-01	9.827E-01	9.893E-01						
4	571.7	9.82	2.760E+00	6.983E-01	2.641E-02	5.223E-03	5.318E-01	
5.427E-01	9.632E-01	9.682E-01						
5	567.6	9.76	2.683E+00	7.747E-01	2.747E-02	5.574E-03	5.959E-01	
6.085E-01	9.570E-01	9.611E-01						
6	564.3	9.70	2.620E+00	8.359E-01	2.838E-02	5.857E-03	6.455E-01	
6.592E-01	9.556E-01	9.590E-01						
7	561.6	9.65	2.568E+00	8.864E-01	2.918E-02	6.093E-03	6.847E-01	
6.992E-01	9.561E-01	9.590E-01						
8	559.3	9.60	2.525E+00	9.292E-01	2.990E-02	6.295E-03	7.164E-01	
7.314E-01	9.573E-01	9.598E-01						
9	557.3	9.56	2.487E+00	9.660E-01	3.056E-02	6.470E-03	7.424E-01	
7.578E-01	9.587E-01	9.610E-01						
10	555.5	9.51	2.454E+00	9.983E-01	3.117E-02	6.624E-03	7.641E-01	
7.798E-01	9.603E-01	9.623E-01						
11	554.0	9.47	2.424E+00	1.027E+00	3.173E-02	6.762E-03	7.824E-01	
7.982E-01	9.618E-01	9.636E-01						
12	552.6	9.43	2.398E+00	1.052E+00	3.226E-02	6.887E-03	7.981E-01	
8.140E-01	9.633E-01	9.649E-01						

Exhibit C

Iteration number 1
 k1c= 1061.0000
 k2c= 5.3500
 k3c= 23.8000
 k4c= 1.5800
 E1c= 74800.0000
 E2c= 74800.0000
 E3c= 54700.0000
 BK3= 95.0000
 BK5= 1100.0000
 AK= 1.5000
 Sinf= .3500
 kd = .0120



1 ETHYL BENZENE DEHYDROGENATION PROGRAM
 ***** REACTOR CALCULATIONS

SUMMARY TABLE FOR PREDICTED PERFORMANCE

FEED ANALYSIS	% MOLE	% WT
BENZENE	.027	.020
TOLUENE	.473	.411
ETHYL BENZENE	99.092	99.168
STYRENE	.408	.401

BED 1

CATALYST TYPE	C-035	(*RELATIVE ACTIVITY =
SIZE(DIA.)	3.30 MM	.130 INCH
VOLUME		
CATALYST	66.3318 M3	***** FT3
HEADSPACE	9.4900 M3	335.09888 FT3
S/O	10.01 M/M	1.70 W/W
LHSV	.73 V/V-HR	.40 W/W-HR
T(IN)	608.00 DEGC	1126.40 DEGF
P(IN)	.70 BAR	10.10 PSIA
T DROP	.26 DEGC	.48 DEGF
P DROP	.1044 BAR	1.51 PSI
CONVERSION	79.42 %M	79.42 %W
SELECTIVITIES		
STYRENE	95.24 %M	93.44 %W
TOLUENE	3.84 %M	3.33 %W
BENZENE	.62 %M	.46 %W

The measured values at 0 days are:
 Conversion= 37.20
 S(Styrene)= 98.30 S(Toluene)= 1.20 S(Benzene)= .50
 DT(Inlet-Outlet)= 48.60

BED 2

CATALYST TYPE	C-035	(*RELATIVE ACTIVITY =
SIZE(DIA.)	3.30 MM	.130 INCH
VOLUME		

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 MC 1700 MAIL ROOM

CATALYST	66.1630 M3	***** FT3
HEADSPACE	12.6400 M3	446.32769 FT3
S/O	10.01 M/M	1.70 W/W
LHSV	.73 V/V-HR	.40 W/W-HR
T(IN)	608.00 DEGC	1126.40 DEGF
P(IN)	.50 BAR	7.30 PSIA
T DROP	.03 DEGC	.05 DEGF
P DROP	.1610 BAR	2.34 PSI
CONVERSION	87.67 %M	87.67 %W
SELECTIVITIES		
STYRENE	93.56 %M	91.79 %W
TOLUENE	5.32 %M	4.62 %W
BENZENE	.70 %M	.52 %W

The measured values at 0 days are:

Conversion= 63.70

S(Styrene)= 97.50 S(Toluene)= 1.90 S(Benzene)= .60

DT(Inlet-Outlet)= 26.30

1 YIELD 82.02 %M 80.46 %W
ETHYL BENZENE DEHYDROGENATION PROGRAM
***** REACTOR CALCULATIONS

SUMMARY TABLE FOR PREDICTED PERFORMANCE

FEED ANALYSIS	% MOLE	% WT
BENZENE	.027	.020
TOLUENE	.473	.411
ETHYL BENZENE	99.092	99.168
STYRENE	.408	.401

BED 1

CATALYST		
TYPE	C-035	(*RELATIVE ACTIVITY =
SIZE(DIA.)	3.30 MM	.130 INCH
VOLUME		
CATALYST	66.3318 M3	***** FT3
HEADSPACE	9.4900 M3	335.09888 FT3
S/O	10.01 M/M	1.70 W/W
LHSV	.73 V/V-HR	.40 W/W-HR
T(IN)	608.00 DEGC	1126.40 DEGF
P(IN)	.70 BAR	10.10 PSIA
T DROP	.26 DEGC	.47 DEGF
P DROP	.1044 BAR	1.51 PSI
CONVERSION	78.96 %M	78.96 %W
SELECTIVITIES		
STYRENE	95.42 %M	93.61 %W
TOLUENE	3.68 %M	3.19 %W
BENZENE	.62 %M	.45 %W

The measured values at 10 days are:

Conversion= 36.90

S(Styrene)= 98.20 S(Toluene)= 1.20 S(Benzene)= .60

DT(Inlet-Outlet)= 48.60

Exhibit D

```

Iteration number      1
k1c=      1061.0000
k2c=       5.3500
k3c=      23.8000
k4c=       1.5800
E1c=      74800.0000
E2c=      74800.0000
E3c=      54700.0000
BK3=       95.0000
BK5=     1100.0000
AK=        1.5000
Sinf=      .3500
kd =       .0120
  
```



ETHYL BENZENE DEHYDROGENATION PROGRAM

1
 ***** REACTOR CALCULATIONS

SUMMARY TABLE FOR PREDICTED PERFORMANCE



FEED ANALYSIS	% MOLE	% WT
BENZENE	.027	.020
TOLUENE	.473	.411
ETHYL BENZENE	99.092	99.168
STYRENE	.408	.401

BED 1

CATALYST TYPE	C-035	(*RELATIVE ACTIVITY =
SIZE(DIA.)	3.30 MM	.130 INCH
VOLUME		
CATALYST	33.5312 M3	***** FT3
HEADSPACE	9.4900 M3	335.09888 FT3
S/O	10.01 M/M	1.70 W/W
LHSV	1.45 V/V-HR	.80 W/W-HR
T(IN)	608.00 DEGC	1126.40 DEGC
P(IN)	.70 BAR	10.10 PSIA
T DROP	63.93 DEGC	115.08 DEGC
P DROP	.0642 BAR	.93 PSI
CONVERSION	35.26 %M	35.26 %W
SELECTIVITIES		
STYRENE	97.64 %M	95.79 %W
TOLUENE	1.63 %M	1.42 %W
BENZENE	.55 %M	.40 %W

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 TC 1700 MAIL ROOM

The measured values at 0 days are:
 Conversion= 37.20
 S(Styrene)= 98.30 S(Toluene)= 1.20 S(Benzene)= .50
 DT(Inlet-Outlet)= 48.60

BED 2

CATALYST TYPE	C-035	(*RELATIVE ACTIVITY =
SIZE(DIA.)	3.30 MM	.130 INCH
VOLUME		

CATALYST	32.8006 M3	***** FT3
HEADSPACE	.0000 M3	.00000 FT3
S/O	10.01 M/M	1.70 W/W
LHSV	1.48 V/V-HR	.82 W/W-HR
T(IN)	608.00 DEGC	1126.40 DEGF
P(IN)	.50 BAR	7.30 PSIA
T DROP	42.21 DEGC	75.99 DEGF
P DROP	.0409 BAR	.59 PSI
CONVERSION	58.49 %M	58.49 %W
SELECTIVITIES		
STYRENE	97.22 %M	95.37 %W
TOLUENE	2.04 %M	1.77 %W
BENZENE	.52 %M	.39 %W

The measured values at 0 days are:

Conversion= 63.70

S(Styrene)= 97.50 S(Toluene)= 1.90 S(Benzene)= .60

DT(Inlet-Outlet)= 26.30

1	YIELD	56.87 %M	55.79 %W
*****	REACTOR CALCULATIONS	ETHYL BENZENE DEHYDROGENATION PROGRAM	

SUMMARY TABLE FOR PREDICTED PERFORMANCE

FEED ANALYSIS	% MOLE	% WT
BENZENE	.027	.020
TOLUENE	.473	.411
ETHYL BENZENE	99.092	99.168
STYRENE	.408	.401

BED 1

.926)	CATALYST		
	TYPE	C-035	(*RELATIVE ACTIVITY =
	SIZE(DIA.)	3.30 MM	.130 INCH
	VOLUME		
	CATALYST	33.5312 M3	***** FT3
	HEADSPACE	9.4900 M3	335.09888 FT3
	S/O	10.01 M/M	1.70 W/W
	LHSV	1.45 V/V-HR	.80 W/W-HR
	T(IN)	608.00 DEGC	1126.40 DEGF
	P(IN)	.70 BAR	10.10 PSIA
	T DROP	63.19 DEGC	113.75 DEGF
	P DROP	.0642 BAR	.93 PSI
	CONVERSION	34.87 %M	34.87 %W
	SELECTIVITIES		
	STYRENE	97.69 %M	95.84 %W
	TOLUENE	1.58 %M	1.37 %W
	BENZENE	.55 %M	.41 %W

The measured values at 10 days are:

Conversion= 36.90

S(Styrene)= 98.20 S(Toluene)= 1.20 S(Benzene)= .60

DT(Inlet-Outlet)= 48.60

Exhibit E

Membrane Design - Mass and Heat Balances

Reactor Dimensions

Stage 1

Inner ID	1.6	m	5.2493438	ft		
Outer ID	3.14	m	10.301837	ft		
Length	11.57	m	37.96	ft		
Bed voidage	0.3					
Bed volume	66.33	m ³	2342.4882	ft ³	17523.03	gal
Bed particle volume	46.43	m ³	1639.7418	ft ³	12266.12	gal
Packing density	570	kg/m ³	35.583943	lb/ft ³		
Particle density	1900	kg/m ³	118.61314	lb/ft ⁴		
Catalyst mass	37809	kg	83354.967	lb		



Inlet/Outlet Conditions

Inlet

Outlet

Temperature	608	C			567.1	C	
Pressure	0.691	Atm	10.15	psia	0.622	Atm	
Oil mass flow rate	11.722	kg/s	25.84308	lb/s	11.65	kg/s	
Steam to oil ratio	1.7	kg/kg-oil	10.01	m/m			
Steam flow rate	19.9277778	kg/s	43.933236	lb/s	19.863	kg/s	86.17%
Total feed flow rate	31.650	kg/s	69.776317	lb/s	31.648	kg/s	
Vol. Feed flow rate	26.789	sm ³ /s	946.02716	scfs	2515	l/h	
Ethyl benzene	99.09%	%m	0.1096	kmol/s	0.0455	kmol/s	3.551%
Styrene	0.41%	%m	0.0005	kmol/s	0.0628	kmol/s	4.902%
Toluene	0.47%	%m	0.0005	kmol/s	0.0017	kmol/s	0.133%
Benzene	0.03%	%m	0.0000	kmol/s	0.0006	kmol/s	0.049%
Total oil	100.00%	%m	0.1106	kmol/s	0.1106	kmol/s	8.636%
Hydrogen	0.00%	%m	-	kmol/s	0.0665	kmol/s	5.192%
Equilibrium Π_{ci} , K	0.0446	Π_{ci}	0.1152	K	38.7%	Π_{ci}/K	
With x% H ₂ removal	0.0321	Π_{ci}	29%	H ₂ removal	27.9%	Π_{ci}/K	



Mass Performance

EB Conversion	0.00%	%in	58.50%	%out	58.50%	%delta	
Styrene selectivity	97.22%	%M	95.69%	%W			
Toluene selectivity	1.84%	%M	0.51%	%W			
Benzene selectivity	0.94%	%M	1.47%	%W			
H ₂ produced	0.06649	kmol/s	0.293179	lb/s	0.13298	kg/s	

Heat performance

Styrene rxn enthalpy	124808	kJ/kmol	53.66	MBTU/lbmol	EB->Sty+H ₂	
Toluene rxn enthalpy	-63385	kJ/kmol	-27.25	MBTU/lbmol	EB+ 2H ₂ O->To+CO ₂ +2H ₂	
Benzene rxn enthalpy	101809	kJ/kmol	43.77	MBTU/lbmol	EB+2H ₂ O->Be+CH ₄ +CO ₂ +2H ₂	
Water heat capacity	2210.7000	J/kg.K	0.5280145	BTU/lb.F		
EB heat capacity	2780.0000	J/kg.K	0.6639889	BTU/lb.F		
Sty Heat capacity	2590.0000	J/kg.K	0.6186083	BTU/lb.F		
Tol Heat capacity	2686.0000	J/kg.K	0.6415375	BTU/lb.F		
Ben Heat capacity	2570.0000	J/kg.K	0.6138314	BTU/lb.F		
Heat duty	3137.25232	kW	10704.707	MBTU/h		
Temperature rise	40.94	K	73.695211	F	104.49	K

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TC 1700 MAIL ROOM

Membrane performance

Max Hydrogen flux needed	0.06470906	kg/s	0.1426591	lb/s	49%	of produced
Max Oxygen flux needed	0.51767244	kg/s	1.1412726	lb/s	0.016177	kmol/s
Membrane permeability	0.012	sm ³ /m ² .s.Atm	0.5	exponent		
H ₂ partial pressure	5.19%	%m	0.03228	Atm		
Actual Area needed	200.5	m ²	2158	ft ²		
Porous tube diameter	0.0254	m	0.0833333	ft	1	in
Area per tube	0.923	m ²	9.9	ft ²		
Number of tubes needed	217	tubes				